

## Multireference F12 Coupled Cluster Theory

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We report development and implementation of explicitly correlated multireference coupled cluster methods that include configurations explicitly depending on the correlation factor of Slater type geminal. Namely, Brillouin Wigner [1] and Mukherjee's [2] MR CC approaches with single and double excitations are extended in this manner. Additional configurations that include pair functions with the correlation factor are generated separately for each reference determinant [3] similarly as in CCSD-F12 [4]. The performance is shown for model systems and small polyatomic molecules using variants with full optimization of the geminal amplitudes, partial optimization of those amplitudes, and fixed amplitudes corresponding to the theoretical cusp conditions. Like in single reference methods, results show a dramatically improved convergence of total energies towards the complete basis set limit as compared to a conventional MR CC approach.

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